COMPONENTS:

- (1) Potassium iso.butanoate (potassium
 iso.butyrate);
 (i.C₄H₇O₂)K; [19455-20-0]
- (2) Sodium iso-butanoate (sodium iso-butyrate); (1.C₄H₇O₂)Na; [996-30-5]

EVALUATOR:

Schiraldi, A., Dipartimento di Chimica Fisica Universita' di Pavia (ITALY).

CRITICAL EVALUATION:

This system was studied only by Sokolov and Pochtakova (Ref. 1) who suggested the phase diagram to be of the eutectic type, the invariant point occurring at 521 K (248 $^{\circ}$ C) and $100\mathbf{x}_{1}=7.5$.

Component 1, however, forms liquid crystals. Therefore the temperature of 633 K (360 $^{
m O}$ C) given in Ref. 1 should be identified with the clearing (and not the fusion) temperature of this component, and compared with the $T_{
m clr}(1)$ value (625.6+0.8 K) reported in Table 2.

For the same component, three phase transition temperatures are quoted in Ref. 1 from Ref. 2, i.e., 621, 546, and 481 K, the second of which can be reasonably identified with the fusion temperature [$T_{\rm fus}(1)$ = 553.9+0.5 K] listed in Preface, Table 2. Consequently: (i) the transition temperature at 621 K (if actually existing) might correspond to some kind of transformation (undetected by DSC, see Preface, Table 2) within the liquid crystal field; and (ii) only the transition at 481 K should correspond to a solid state transformation, although the latter figure is almost 60 K higher than the single $T_{\rm trs}(1)$ value (424+3 K) listed in Table 2 of the Preface.

Concerning component 2, the fusion temperature of 535 K (262 °C; Ref. 1) is in reasonable agreement with that (526.9 ± 0.7 K) reported in Table 2 of the Preface. In this Table, however, no mention is made of other phase transformations, although three solid state transitions are quoted for this component in Ref. 1 (from Ref. 2), at 493, 364, and 340 K (220, 91, and 67 °C), respectively. Duruz et al. (Ref. 3) report in turns fusion at 527 K (in agreement with the fusion temperature from Table 2), and solid state transitions at 493 K (in agreement with the highest transition temperature from Ref. 2), and at 468 K (a figure which has no correspondence in Ref. 2). Finally, Ferloni et al. (Ref. 4) are inclined to think that Sokolov's transformation at 340 K (Ref. 2) actually represents a transition of a hydrated form of the salt.

In the evaluator's opinion, a re-investigation of the phase relations in solid sodium iso.butanoate would be desirable. At any rate, the phase diagram suggested by Sokolov and Pochtakova (Ref. 1) has to be modified (due to the occurrence of liquid crystals in component 1) with reference to Schemes A.1, or A.3, of the Preface according to the kind of solid state miscibility between components, the eutectic point actually being an M'E point.

REFERENCES:

- (1) Sokolov, N.M.; Pochtakova, E.I. Zh. Obshch. Khim. 1960, 30, 1405-1410 (*); Russ. J. Gen. Chem. (Engl. Transl.) 1960, 30, 1433-1437.
- (2) Sokolov, N.M. Tezisy Dokl. X Nauch. Konf. S.M.I. 1956.
- (3) Duruz, J.J.; Michels, H.J.; Ubbelohde, A.R. Proc. Roy. Soc. London 1971, A 322, 281-299.
- (4) Ferloni, P.; Sanesi, M.; Tonelli, P.L.; Franzosini, P. Z. Naturforsch. 1978, A 33, 240-242.

COMPONENTS:

- (1) Potassium iso.butanoate (potassium
 iso.butyrate);
 (i.C₄H₇O₂)K; [19455-20-0]
- (2) Sodium iso.butanoate (sodium iso.butyrate); (1.C₄H₇O₂)Na; [996-30-5]

ORIGINAL MEASUREMENTS:

Sokolov, N.M.; Pochtakova, E.I. Zh. Obshch. Khim. 1960, 30, 1405-1410 (*); Russ. J. Gen. Chem. (Engl. Transl.) 1960, 30, 1433-1437.

VARIABLES:

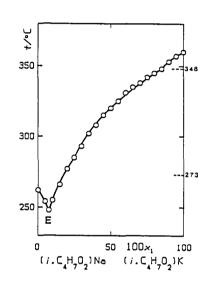
Temperature.

PREPARED BY:

Baldini, P.

EXPERIMENTAL VALUES:

EXPERTMENTAL		VALUES:
t/°C	T/K ^a	100 x 1
262	535	0
254	527	5
248	521	7.5
255	528	10
266	539	15
277	550	20
285	558	25
293	566	30
302	575	35
308	581	40
315	588	45
320	593	50
325	598	55
331	604	60
335	608	65
338	611	70
342	615	75
345	618	80
348	621	85
353	626	90
357	630	95
360	633	100



Characteristic point(s): Eutectic, E, at 248 °C and $100x_1 = 7.5$ (authors).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Visual polythermal analysis.

REFERENCES:

- (1) Sokolov, N.M.
 Zh. Obshch. Khim. 1954, 24, 1150-1156.
- (2) Sokolov, N.M. Tezisy Dokl. X Nauch. Konf. S.M.I. 1956 (this is Ref. 6 in the original paper, and not Ref. 5 as erroneously quoted in the text; compiler).

SOURCE AND PURITY OF MATERIALS:

Both components were prepared from commercial "pure" grade iso.butanoic acid, distilled before use, and the proper "chemically pure" hydrogen carbonate (Ref. 1); then recrystallized from n-butanol. Component 1 undergoes phase transitions at $t_{\rm trs}(1)/{}^{\rm C}$ c= 208, 273, 348 (Ref. 2). Component 2 undergoes phase transitions at $t_{\rm trs}(2)/{}^{\rm C}$ c= 67, 91, 220 (Ref. 2).

ESTIMATED ERROR:

Temperature: accuracy probably +2 K (compiler).

a T/K values calculated by the compiler.